Amendments to the Claims

This listing of claims will replace all prior versions and listings of claims in the application:

Listing of Claims:

1. (currently amended) A method for predicting pharmacokinetic properties of molecules comprising the steps of:

(a) preparing 2D-structures of molecules used as a training set;

(b) constructing a 2D-fingerprint by counting the number of structural descriptors that may ~~potentially~~ relate to a pharmacokinetic property of a molecule set forth in the training set, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;

(c) analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and

(d) calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.

2. (original) A method of Claim 1, wherein the pharmacokinetic property is absorption.

3. (withdrawn) A method of Claim 1, wherein the pharmacokinetic property is distribution.

4. (wthdrawn) A method of Claim 1, wherein the pharmacokinetic property is metabolism

5. (withdrawn) A method of Claim 1, wherein the pharmacokinetic property is excretion.

6. (currently amended) A method of Claim 1, wherein the internally developed macro comprises the macro script 2dfp.spl or 2dfp_abs.spl, written in a language known as SYBYL™ Programming Language (SPL).

7. (currently amendedl) A system for predicting pharmacokinetic properties of molecules comprising:

(a) means for preparing 2D-structures of molecules used as a training set;

(b) means for constructing a 2D-fingerprint by counting the number of structural

descriptors that may ~~potentially~~ relate to a pharmacokinetic property of a molecule set forth in the training set wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;

(c) means for analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and

(d) means for calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.